M-METHYLPHENETHYL ALCOHOL

Other names: Phenethyl alcohol, m-methyl-
m-Methylphenethyl alcohol
2-m-Tolylethanol
Inchi: InChI=1S/C9H12O/c1-8-3-2-4-9(7-8)5-6-10/h2-4,7,10H,5-6H2,1H3
InchiKey: KWHVBVJDKLSOTB-UHFFFAOYSA-N
Formula: C9H12O
SMILES: Cc1cccc(CCO)c1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
af	0.6388		Cheméo Relay (1.0)
gf	-9.14	kJ/mol	Joback Method
hf	-166.57	kJ/mol	Cheméo Relay (1.0)
hfus	16.81	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-1.24		Cheméo Relay (1.0)
logp	1.530		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	515.70	K	NIST Webbook
tc	739.39	K	Cheméo Relay (1.0)
tf	238.36	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.45	J/mol×K	529.16	Joback Method
cpg	277.78	J/mol×K	561.83	Joback Method
cpg	288.52	J/mol×K	594.49	Joback Method
cpg	298.68	J/mol×K	627.16	Joback Method
cpg	308.29	J/mol×K	659.82	Joback Method

cpg	317.36	J/mol×K	692.49	Joback Method
cpg	325.92	J/mol×K	725.15	Joback Method
dvisc	0.0098792	Pa×s	290.95	Joback Method
dvisc	0.0030353	Pa×s	330.65	Joback Method
dvisc	0.0012010	Pa×s	370.35	Joback Method
dvisc	0.0005687	Pa×s	410.05	Joback Method
dvisc	0.0003073	Pa×s	449.76	Joback Method
dvisc	0.0001835	Pa×s	489.46	Joback Method
dvisc	0.0001184	Pa×s	529.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1875894&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume